Large scale simulations with parallel annealing algorithm

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DIONICOS

RSF | Russian Science Foundation

Grid-2018, Dubna, 2018-09-11

Large scale simulations with parallel annealing algorithm

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RSCF 14-21-11058 and DIONICOS

Grid-2018, Dubna, 2018-09-11

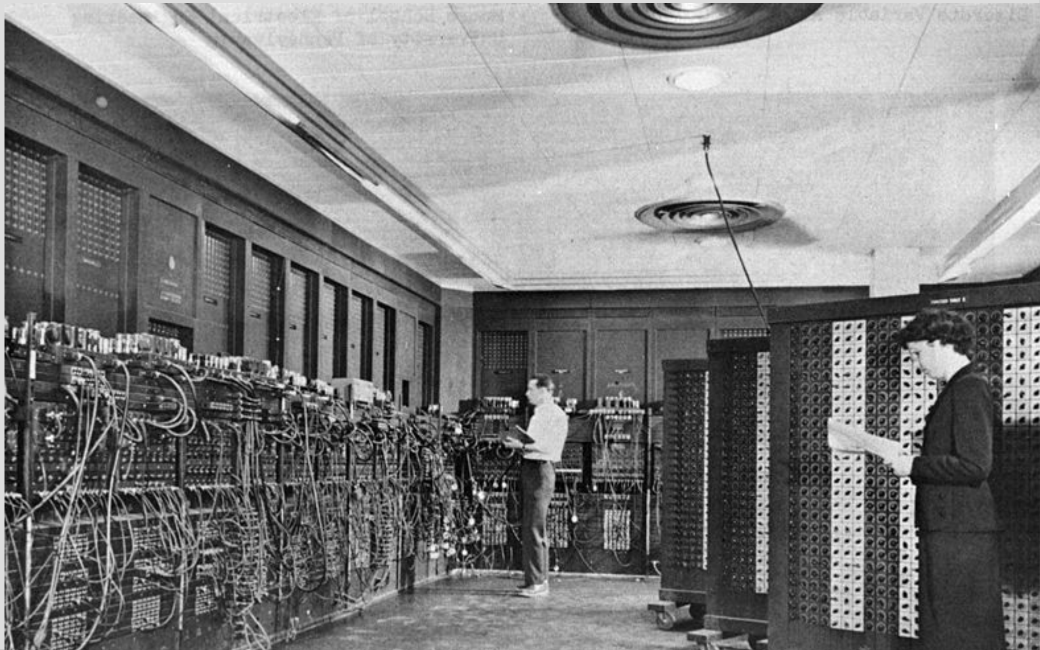
ЭВМ and Supercomputers

XX century - fall of 40th – beginning of 50th:

- nuclear project (hudrodynamics)
- Monte Carlo method - von Neumann, Ulam, Metropolis-Rosenblut^2-Teller^2
- Fermi-Pasta-Ulam problem
- Random Number Problem – von Neumann, Lehmer

МЭСМ, 1950

ENIAC, 1944



ЭВМ and Supercomputers

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- ***Lehmer talk at Symposium*** ***on Large-Scale Digital Calculating***

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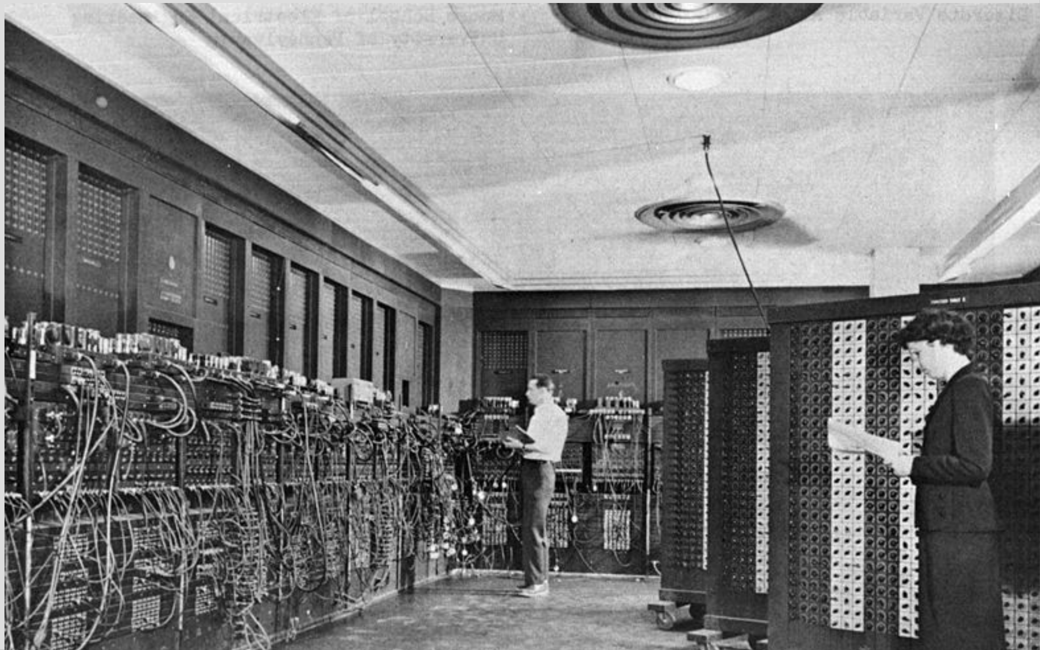
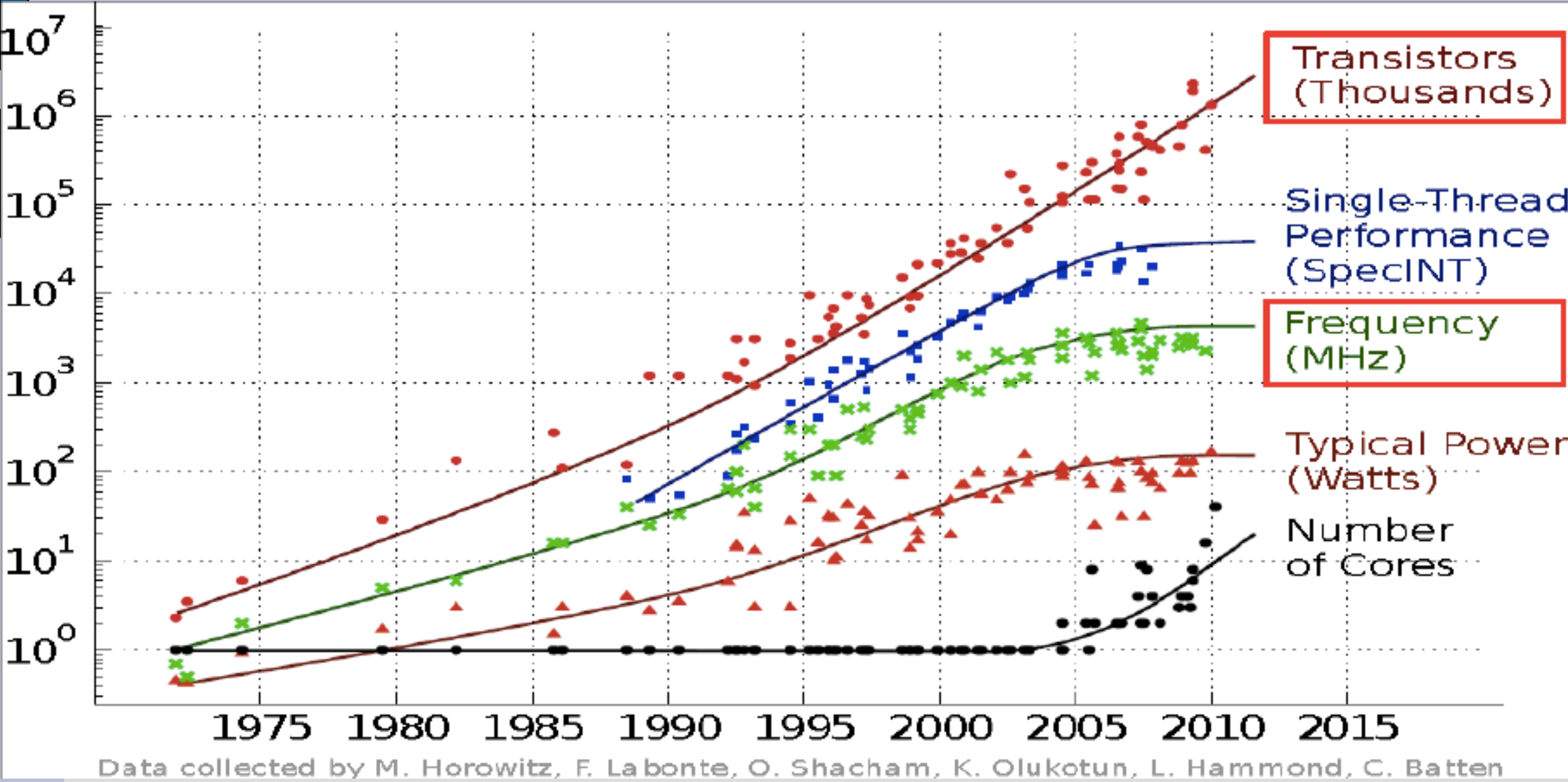
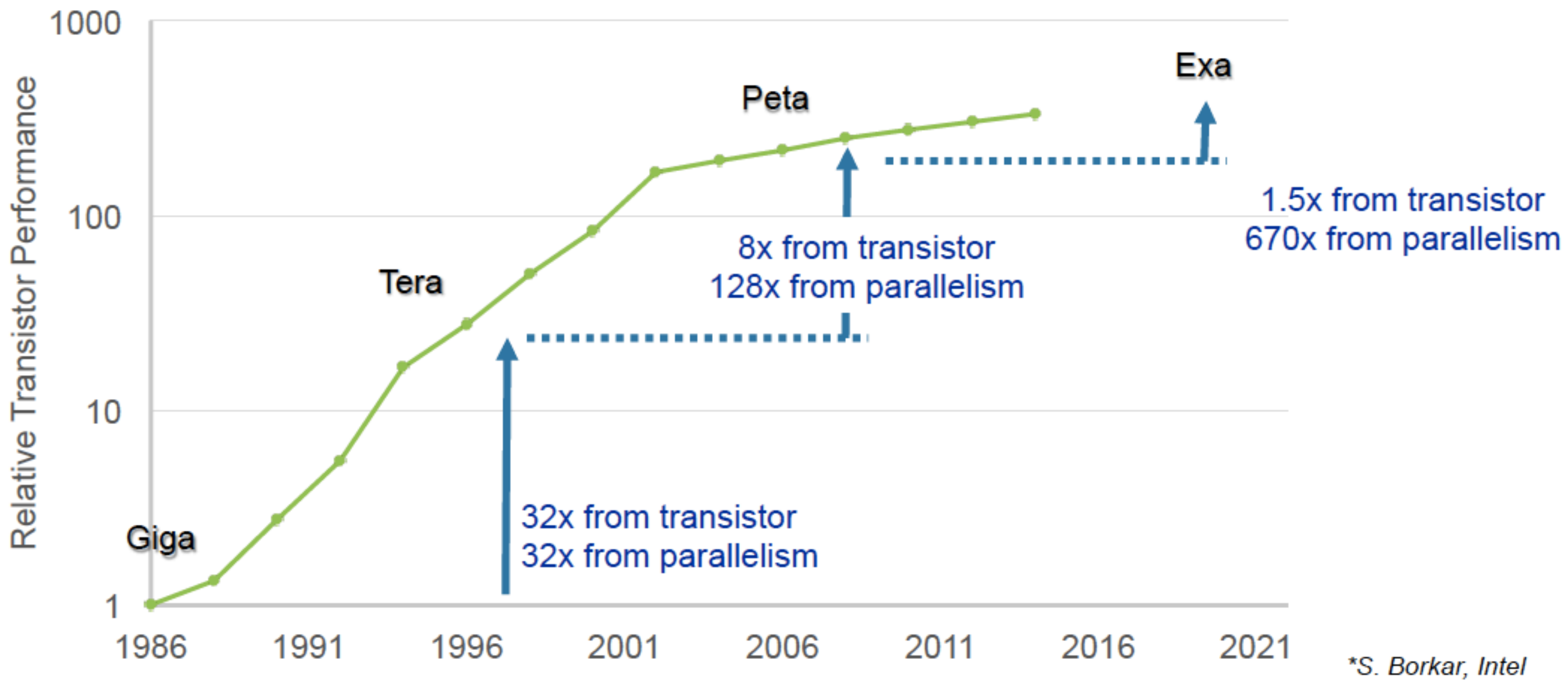


Large scale simulations with parallel annealing algorithm

Moore's law – saturation?
Or something new happens?



From Giga to Exa, via Tera & Peta*



*S. Borkar, Intel

Performance from parallelism

From J. Messina, 31 July, 2016 (ECP director, ANL)

Main goal

The big challenge for scientific computing is to develop algorithms and computational frameworks that use the parallel hardware efficiently.

There are two approaches:

- Develop a universal framework which is potentially is fully scalable;
- Invent an algorithm which is efficient for the particular set of problems.

Examples

There are two approaches:

- *Develop a universal framework which is potentially is fully scalable;*

For example, Parallel Discrete Event Simulation
(talk by Lilia Ziganurova on Friday)

- *Invent an algorithm which is efficient for the particular set of problems*

For example, Population Annealing
(this talk).

Population Annealing algorithm

1. The population annealing algorithm is designed for study systems with rough free-energy landscapes (spin glasses, optimization problems…).
2. Combines the power of the known efficient algorithms - simulated annealing, Boltzmann weighted differential reproduction, and sequential Monte Carlo process.
3. Bring the population of replicas to the equilibrium even in the low-temperature region.
4. Provides a very good estimate of the free energy.
5. PopAnn is performed over a large number of replicas with many spin updates, and it is a good candidate for massive parallelism.
6. Efficient parallel implementation – many replicas.

K. Hukushima, Y. Iba, AIP Conf. Proc. **690** 200 (2003)
J. Machta, Phys. Rev. E **82** 026704 (2010)

Population Annealing algorithm by Machta (PAM)

1. Set up an equilibrium ensemble of $R = R_0$ independent copies (replicas) of the system at inverse temperature β_0. Often $\beta_0 = 0$, where this can be easily achieved.
2. To create an approximately equilibrated sample at $\beta_i > \beta_{i-1}$, resample configurations with their relative Boltzmann weight $\tau_i(E_j) = \exp[-(\beta_i - \beta_{i-1})E_j]/Q_i$, where $Q_i = \sum_j \exp[-(\beta_i - \beta_{i-1})E_j]/R_{i-1}$.
3. Update each replica by θ rounds of an MCMC algorithm at inverse temperature β_i.
4. Calculate estimates for observable quantities $\mathcal{O}$ as population averages $\sum_j \mathcal{O}_j / R_i$.
5. Goto step 2 unless the target temperature β_{K-1} has been reached.

J. Machta, Phys. Rev. E **82** 026704 (2010)

Population Annealing algorithm by Machta (PAM)

Partition function ratio $Q(\beta_k, \beta_{k-1})$ is given by

$$Q(\beta_k, \beta_{k-1}) = \frac{\sum_{j=1}^{\tilde{R}_{\beta_k}} \exp\left[-(\beta_{k-1} - \beta_k)E_j\right]}{\tilde{R}_{\beta_k}} \qquad (1)$$

and normalized weights $\tau_j(\beta_k, \beta_{k-1})$ calculated accordingly by

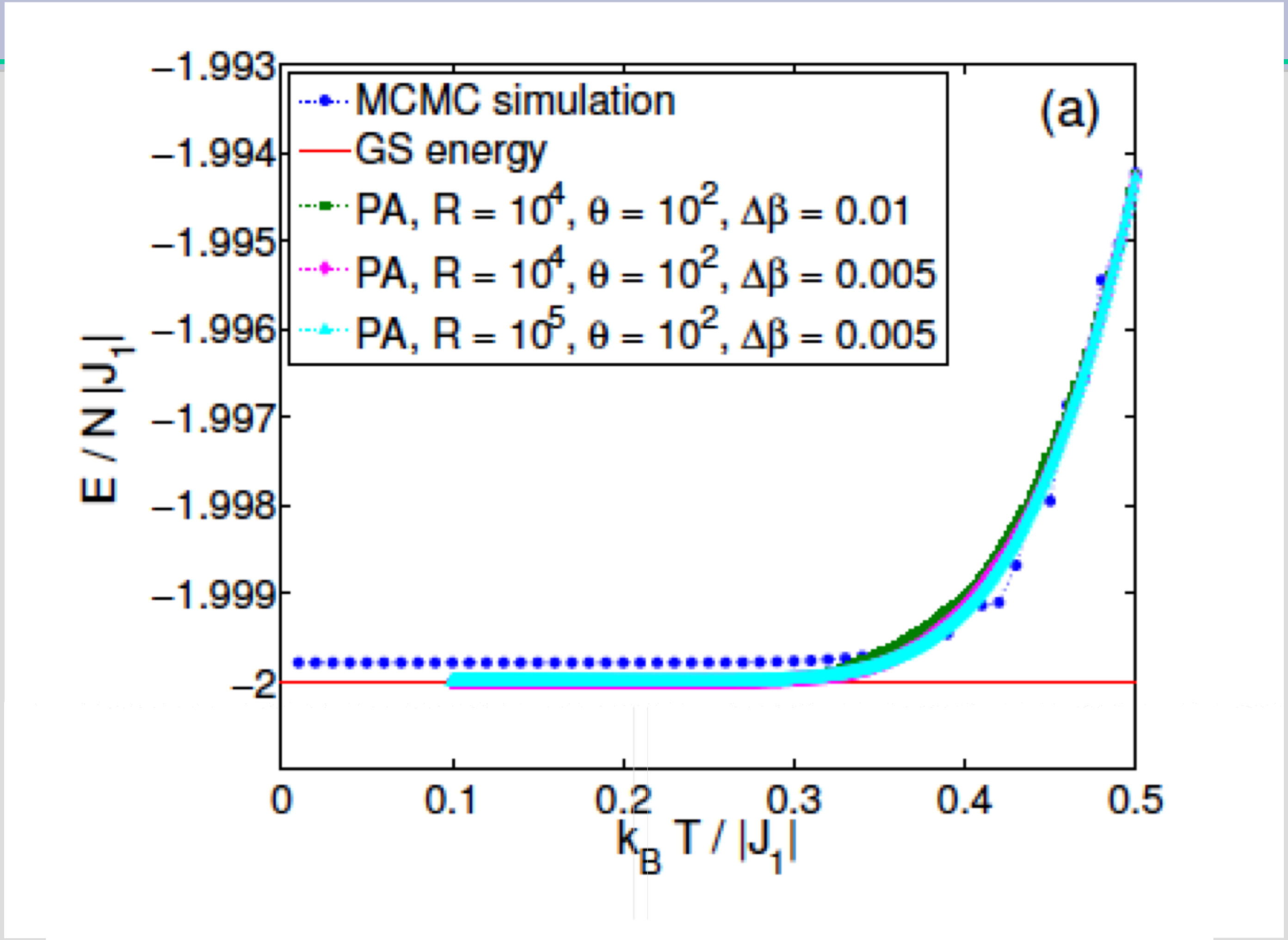
$$\tau_j(\beta_k, \beta_{k-1}) = \frac{\exp\left[-(\beta_{k-1} - \beta_k)E_j\right]}{Q(\beta_k, \beta_{k-1})} \qquad (2)$$

and

$$\tilde{R}_{\beta_k} = \sum_{j=1}^{\tilde{R}_{\beta_k}} \tau_j(\beta_k, \beta_{k-1}). \qquad (3)$$

$$-\beta_k \tilde{F}(\beta_k) = \sum_{i=K}^{k+1} \ln Q(\beta_k, \beta_{k-1}) + \ln \Omega$$

PopAnn, CUDA: frustrated Ising ferromagnet on the stacked triangular lattice



EPJ Web of Conferences **108**, 02016 (2016)

Ising model with Population Annealing

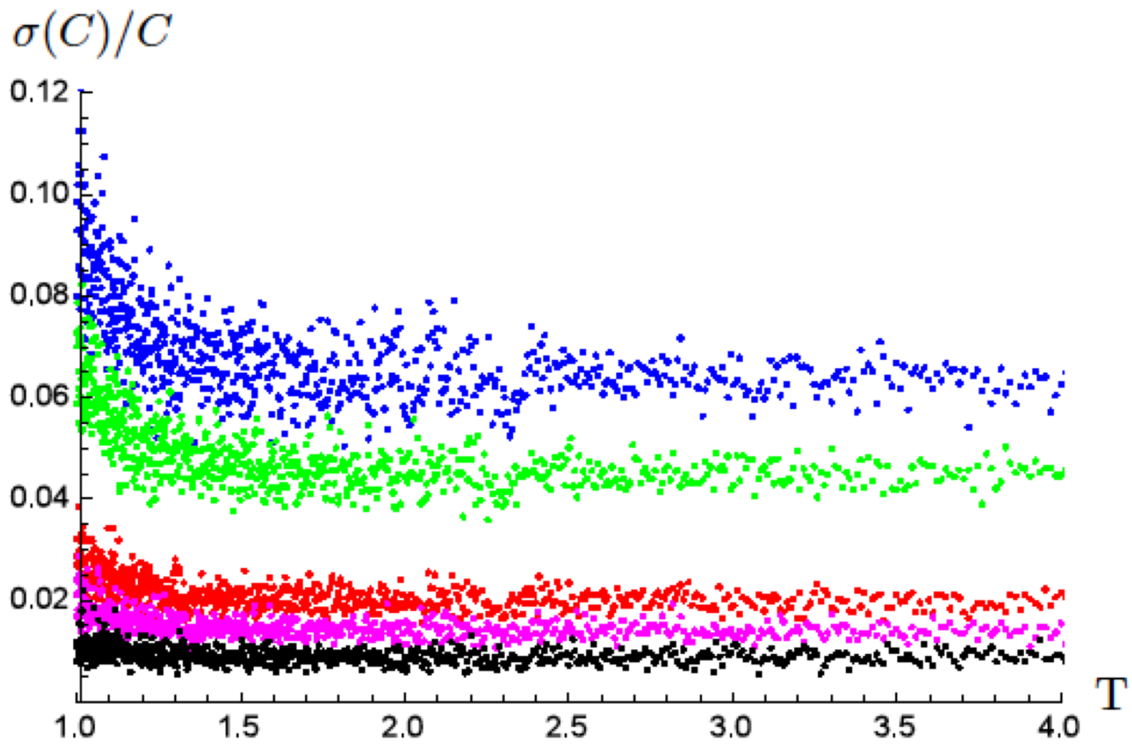


FIG. 5: Relative specific heat errors, $\sigma(C(T))/C(T)$, as a function of the temperature for a different number of replicas R, $R = 500$ - blue, $R = 1000$ - green, $R = 5000$ - red, $R = 10000$ - pink, and $R = 25000$ - black.

Computer Physics Communications (2017)

Potts model with Population Annealing

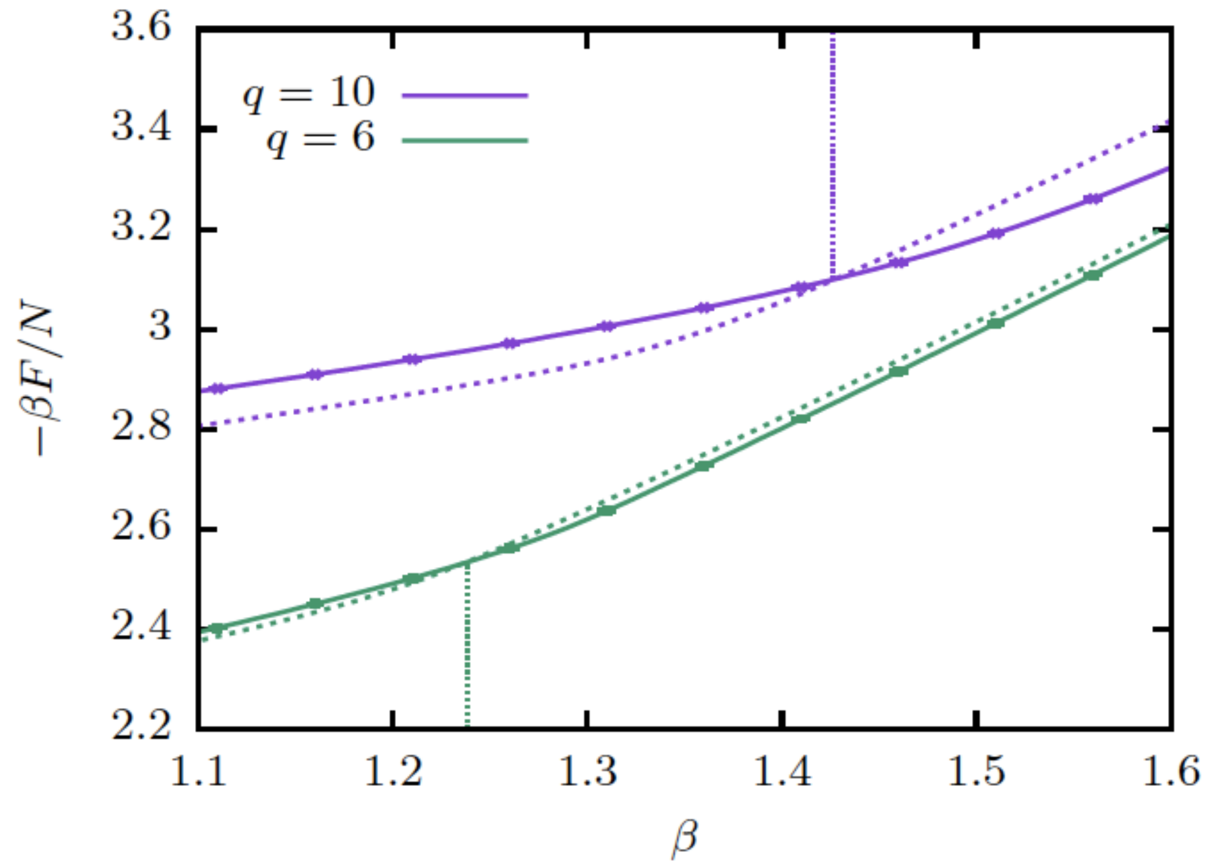
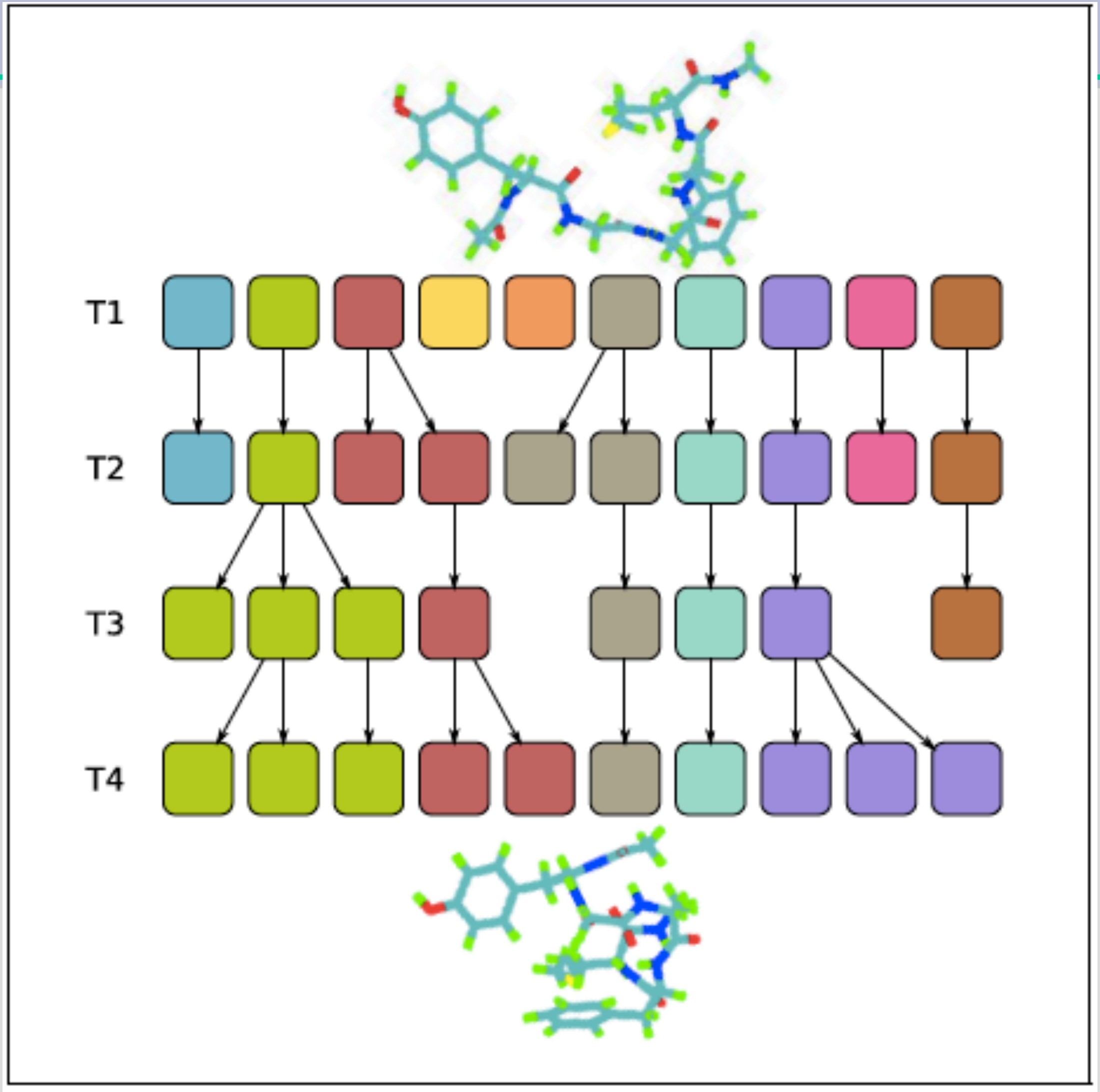


Fig. 2. Metastable free energy for the q-state Potts model with $q = 6$ (green) and $q = 10$ (magenta) for a cooling (solid lines) and a heating (dashed lines) cycle. The vertical dotted lines indicate the locations of the transition points β_t. The lattice size is $L = 32$, and the PA parameters are $\theta = 10$, $R = 10000$, and $\Delta\beta = 0.01$. Taken from Ref. [27].

Eur. Phys. J. Special Topics **226** 595–604 (2017)

Population Annealing for Molecular Dynamics Simulations of Biopolymers



Population Annealing for Molecular Dynamics Simulations of Biopolymers

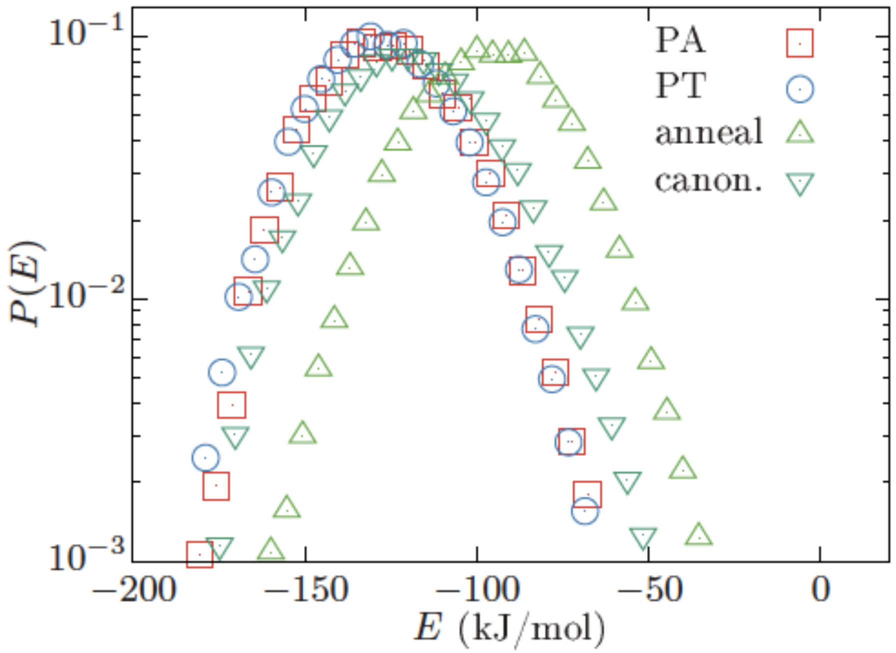
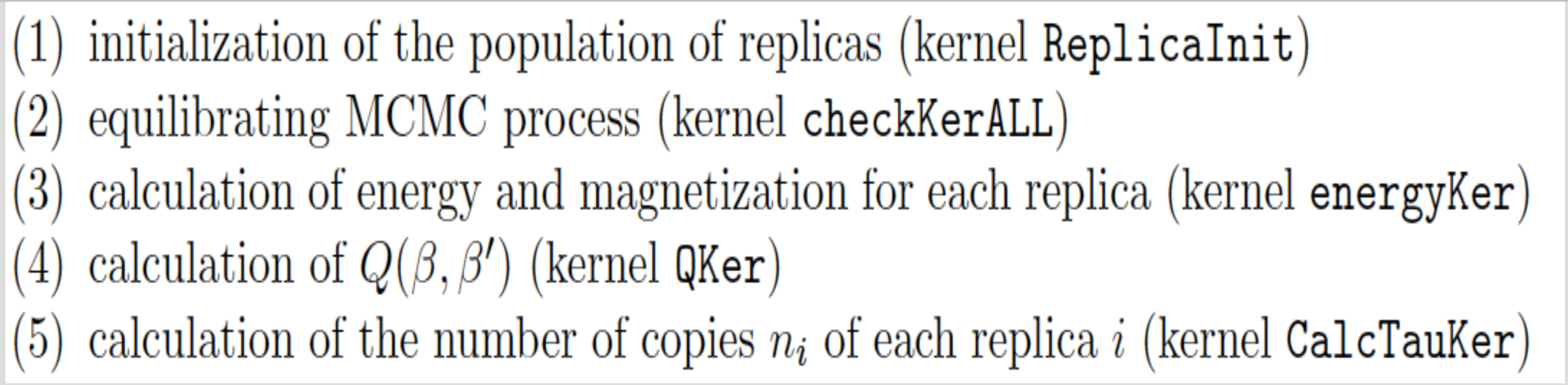
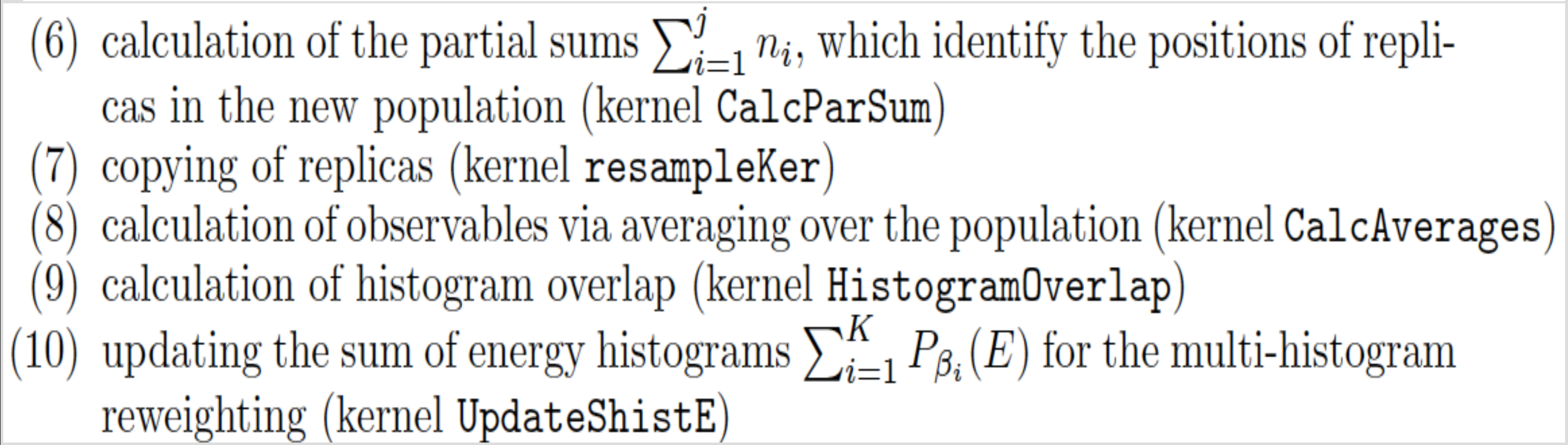


Figure 3: Energy histograms at the lowest temperature, $T = 200$ K, as obtained from the population annealing (PA), parallel tempering (PT), population annealing without resampling ("anneal"), and canonical ("canon.") simulations, respectively.

GPU accelerated PA algorithm



(1) initialization of the population of replicas (kernel `ReplicaInit`)
(2) equilibrating MCMC process (kernel `checkKerALL`)
(3) calculation of energy and magnetization for each replica (kernel `energyKer`)
(4) calculation of $Q(\beta, \beta')$ (kernel `QKer`)
(5) calculation of the number of copies n_i of each replica i (kernel `CalcTauKer`)



(6) calculation of the partial sums $\sum_{i=1}^{j} n_i$, which identify the positions of repli-
cas in the new population (kernel `CalcParSum`)
(7) copying of replicas (kernel `resampleKer`)
(8) calculation of observables via averaging over the population (kernel `CalcAverages`)
(9) calculation of histogram overlap (kernel `HistogramOverlap`)
(10) updating the sum of energy histograms $\sum_{i=1}^{K} P_{\beta_i}(E)$ for the multi-histogram
reweighting (kernel `UpdateShistE`)

GPU accelerated PA algorithm

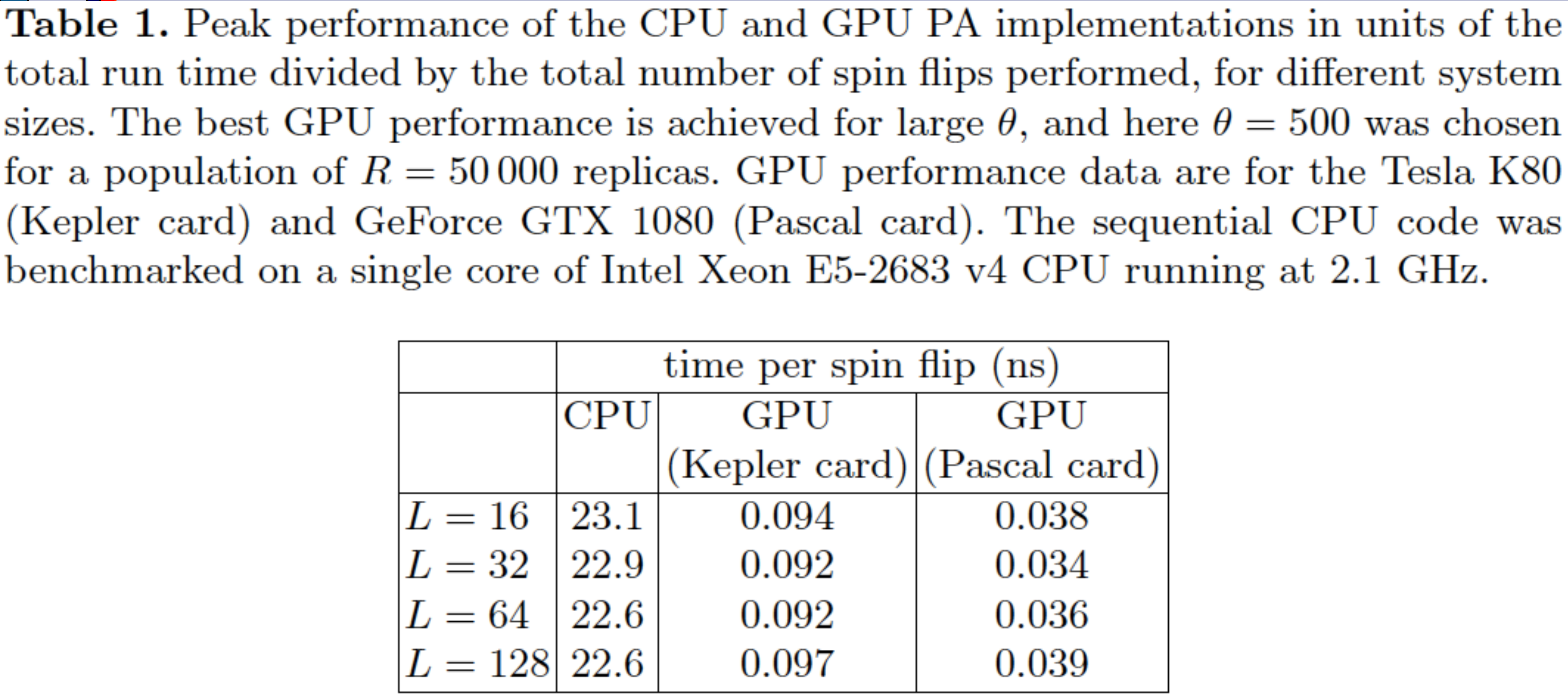


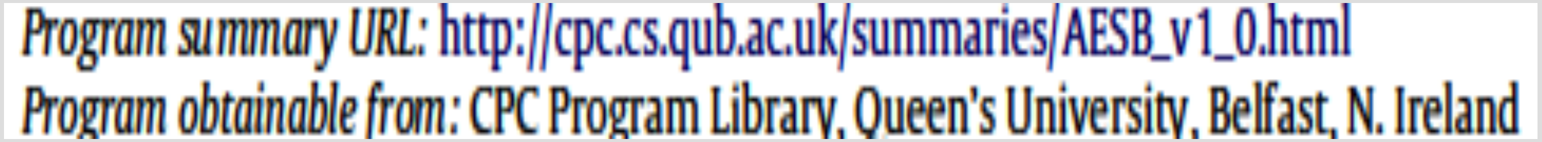
Table 1. Peak performance of the CPU and GPU PA implementations in units of the total run time divided by the total number of spin flips performed, for different system sizes. The best GPU performance is achieved for large θ, and here $\theta = 500$ was chosen for a population of $R = 50\,000$ replicas. GPU performance data are for the Tesla K80 (Kepler card) and GeForce GTX 1080 (Pascal card). The sequential CPU code was benchmarked on a single core of Intel Xeon E5-2683 v4 CPU running at 2.1 GHz.

	time per spin flip (ns)		
	CPU	GPU (Kepler card)	GPU (Pascal card)
$L = 16$	23.1	0.094	0.038
$L = 32$	22.9	0.092	0.034
$L = 64$	22.6	0.092	0.036
$L = 128$	22.6	0.097	0.039

Random Number Generation at “large scale”

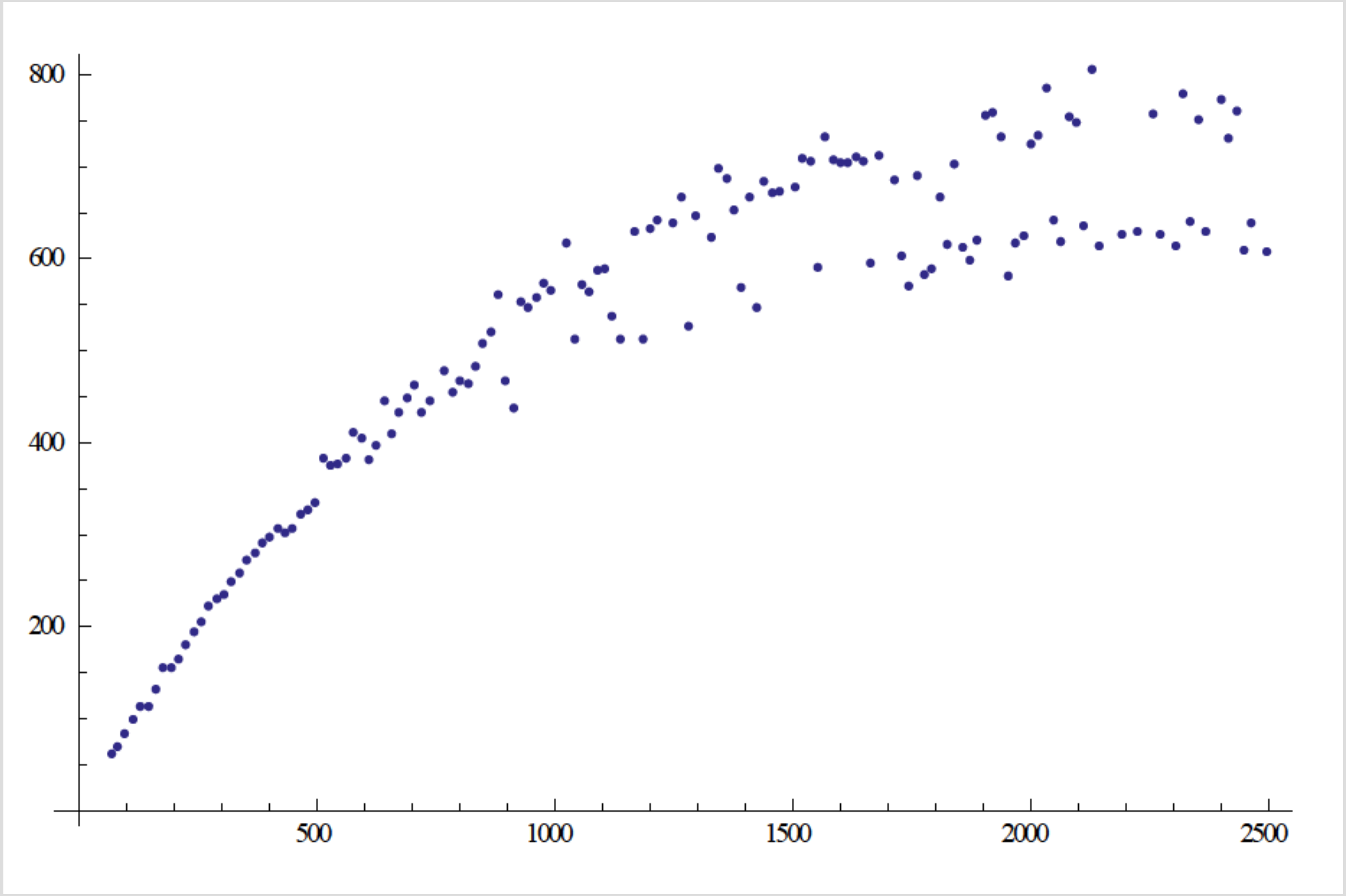
PRAND: GPU accelerated parallel random number generation library:
Using most reliable algorithms and applying parallelism of modern GPUs and CPUs
(L. Barash, LS, **CPC 2014**)

Highlights of PRAND - SSE-accelerated, GPU-accelerated, C, Fortran and CUDA, parallel streams

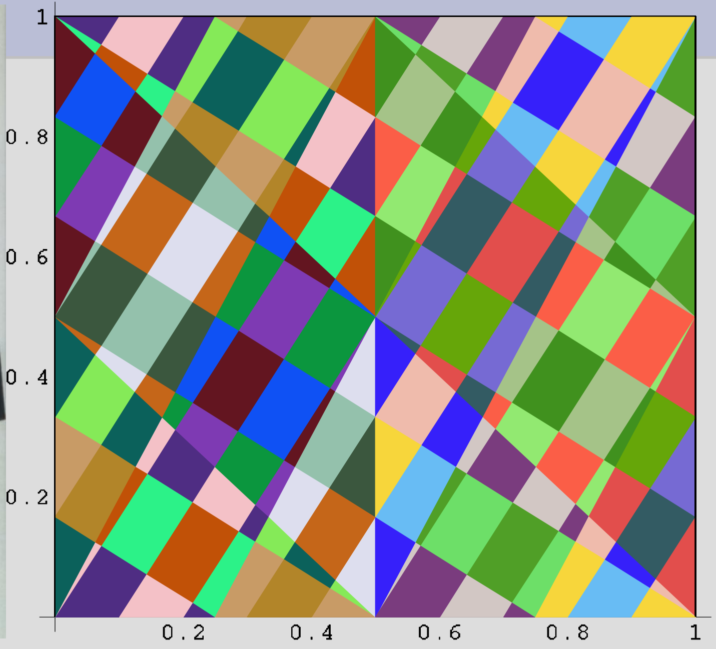

Program summary URL: http://cpc.cs.qub.ac.uk/summaries/AESB_v1_0.html
Program obtainable from: CPC Program Library, Queen's University, Belfast, N. Ireland

MC integral

- MC integral
- Example with 3000 GPGPU (Lomonosov)



PRAND: GM generators (on torus)



Kandisky, Malevich, Barash-Shchur

MPI/GPU PA implementation

Technical problems to solve:

- Load balancing of all GPU nodes with an approximate same number of replicas;
- Minimize large memory exchange between nodes;
- …

Conclusion

- *Population annealing* approach is the promising tool for the number of problems:

• "complex" ground state

• the rough energy landscape

• optimization problems

- *Population annealing* algorithm is the natural candidate for large-scale and *fully scalable simulations* with the *heterogeneous parallelism*.

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Landau Institute for Theoretical Physics

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